

6-Amino-4-hydroxynaphthalene-2-sulfonic acid
90-51-7 | DTXSID0026547

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.89e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.66e-01

Confidence level: 7.57e-01

Nearest Neighbors from the Training Set

Image not found

4-(2-Hydroxyethanesulfonyl)benzene-1-sulfonamide

Measured: 2.49e-02

Predicted: 2.61e-02

Image not found

4-(3-Hydroxypropane-1-sulfonyl)benzene-1-sulfonamide

Measured: 2.58e-02

Predicted: 1.67e-02

Image not found

4-(3-Hydroxy-3-methylbutane-1-sulfonyl)benzene-1-sulfonamide

Measured: 1.14e-02

Predicted: 1.58e-02

Image not found

Benzoic acid, 2-amino-4-sulfo-

Measured: 4.83e-02

Predicted: 3.79e-02